Barcelona Supercomputing Center
Centro Nacional de Supercomputación

EXCELENCIA SEVERO OCHOA

BSC Update: MONARCH model

Oriol Jorba, Sara Basart, Jaime A. Benavides, Francesco Benincasa, Dene Bowdalo, Matthew L. Dawson, Enza Di Tomaso, Jerónimo Escribano, María Gonçalves, Marc Guevara, Elina Karnezi, Martina Klose, Francesca Macchia, Gilbert Montané, Vincenzo Obiso, Miriam Olid, María Teresa Pay, Herve Petetin, Carles Tena and Carlos Pérez García-Pando

Atmospheric Composition Group
Barcelona Supercomputing Center

22/07/2019

11th ICAP WG meeting - Tsukuba (Japan)

Contents

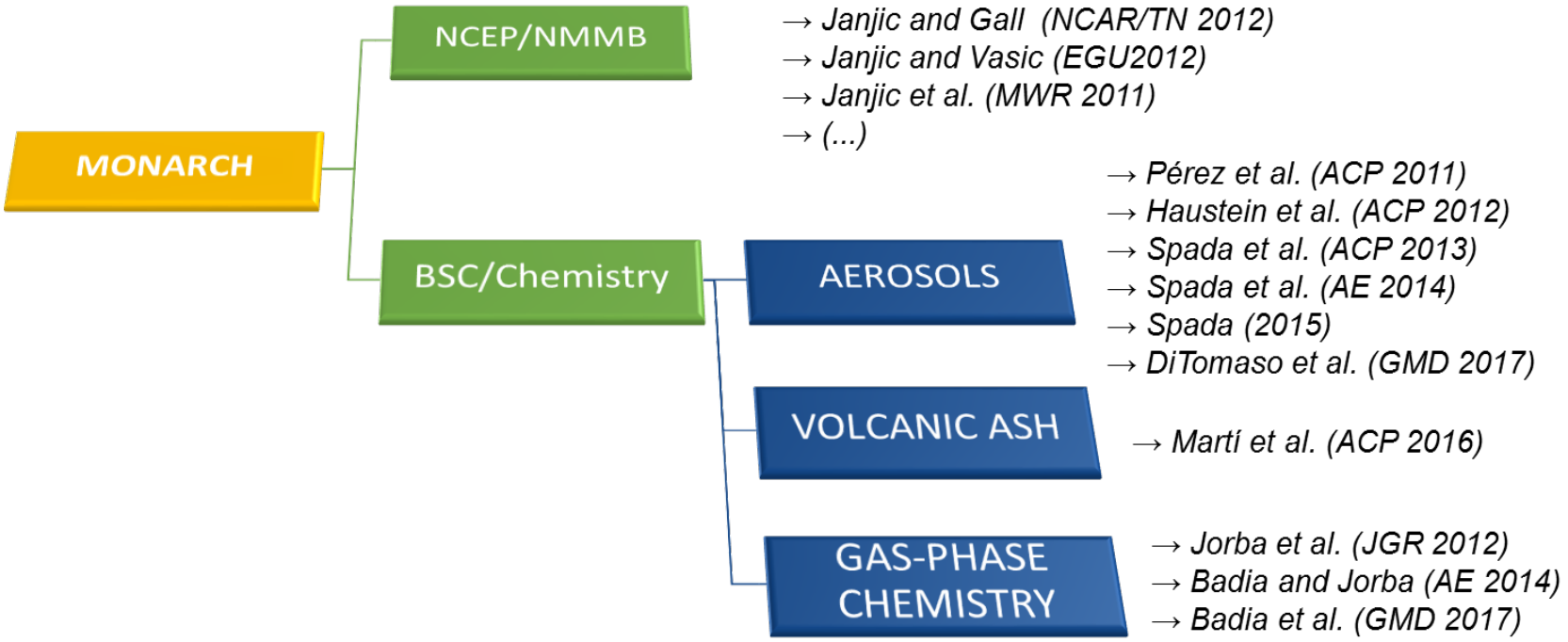
- Overview of the MONARCH model and status of BSC forecast
- Developments:
  - Extending the flexibility of chemistry solvers
  - HERMESv3 emission system
  - GHOST: Globally Harmonised Observational Surface Treatment
- Projects:
  - Sub-contracts with Copernicus Atmophere Monitoring Service
  - Data Assimilation activities
  - FRAGMENT: FRontiers in dust minerAloGical coMposition and its Effects upoN climaTe
  - SDS-WAS

Overview of the MONARCH model and status of BSC forecast

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

The MONARCH model

- ***Multiscale***: global to regional (up to 1km) scales allowed
- Fully ***on-line*** coupling: weather-chemistry feedback processes allowed
- Enhancement with a ***data assimilation*** system



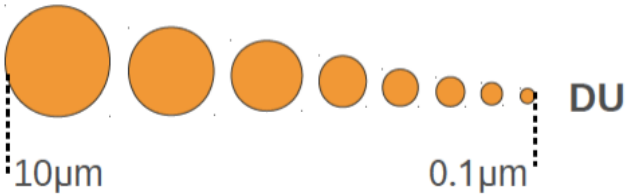
Dust module is known as **NMMB/BSC-Dust**

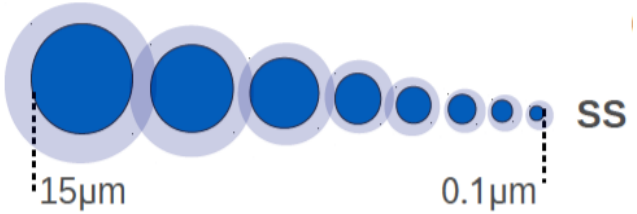
Aerosol Scheme

Sectional

dust (DU)

sea-salt (SS)





Bulk

Black Carbon (BC)

Organic Aerosols (OA)

Primary Organic Aerosols (POA)

Secondary organic aerosols (SOA)

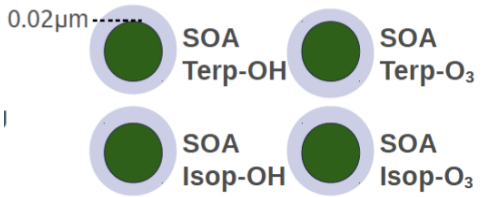
4 gaseous tracers (OH, O3, TERP, ISOP). Online emission (MEGAN)

4 aerosol-phase hydrophilic tracers

2-product scheme of Tsigaridis and Kanakidou (2007)

Oxidation by OH and O3 and gas-particle partitioning

Anthropogenic SOA from Toluene and Xylene under development



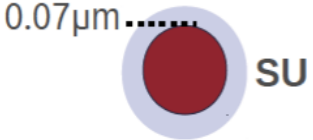
Sulfate (SU):

4 additional prognostic tracers (SO2, DMS, H2O2, H2SO4)

3 online or climatological oxidants (OH, O3, HO2)

gas-phase oxidation of SO2, DMS and H202 by OH

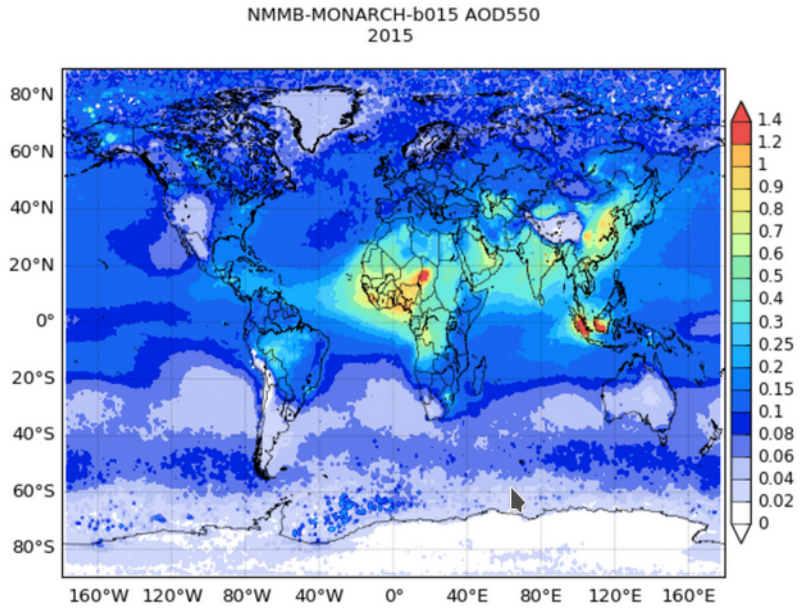
aqueous-phase oxidation by H202 and O3



Nitrate (NO3) and Ammonium (NH4): as calculated by EQSAM thermodynamic equilibrium model but not evaluated yet

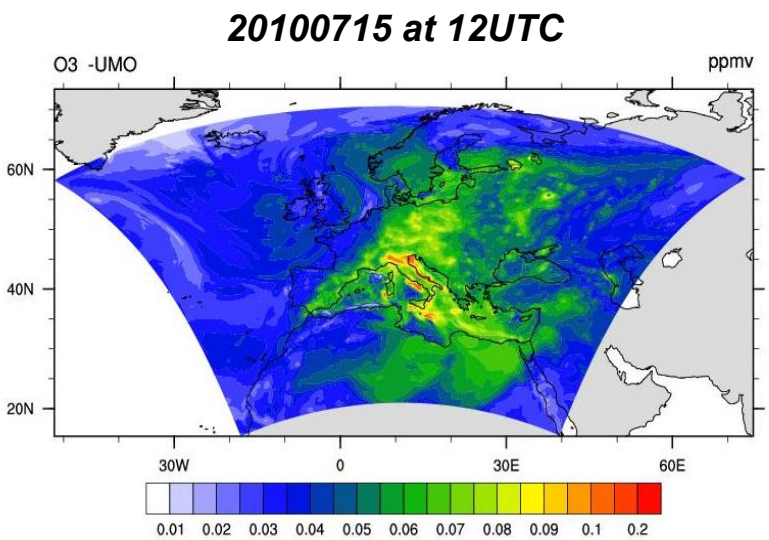
MONARCH forecasts

Global



- ✓ *MONARCH contributes to the **ICAP global forecast aerosol** multi-model ensemble* http://icap.atmos.und.edu

Regional



- ✓ ***BDFC** and **SDS-WAS** dust forecast*
- ✓ *Candidate model **CAMS_50.II***
- ✓ *It will be implemented in*

CALIOPE *(www.bsc.es/caliope) AQ Forecast System for **EU** and **Spain***

And more products in: http://www.bsc.es/ess/

BSC ICAP Current forecasts and plans

CURRENT FORECASTING – DEVELOPED/AVAILABLE – UNDER DEVELOPMENT - PLANNED

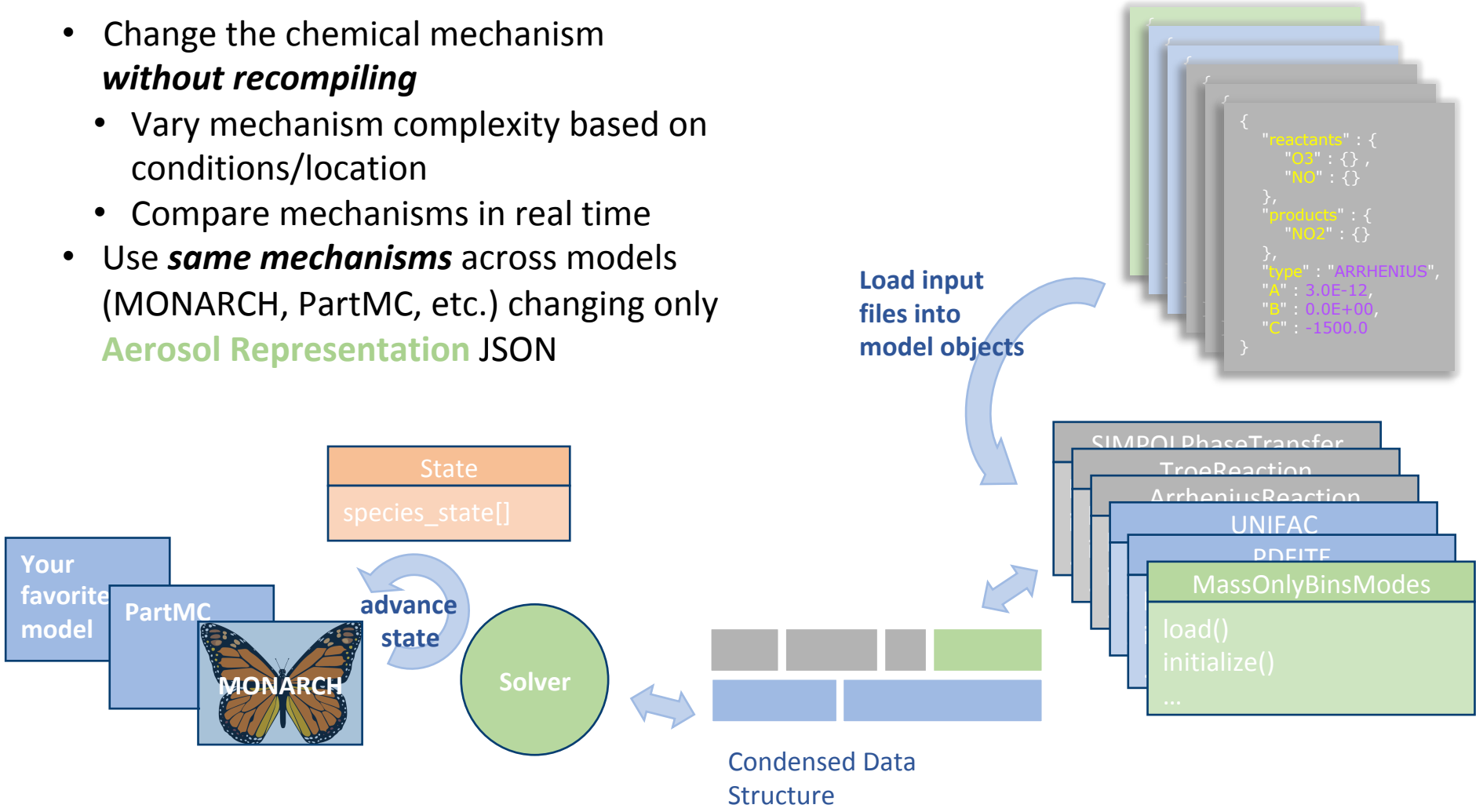
DOMAIN	GLOBAL (ICAP)	REGIONAL North Africa, Middle East and Europe (SDS-WAS)	REGIONAL Europe/Iberian Peninsula/Urban Areas (CALIOPE)
Model	MONARCH	MONARCH	CMAQ (DREAM for dust) MONARCH
Status	QO	O	O
Meteorology	Inline: NMMB	Inline: NMMB	Offline: WRF-ARW Inline: NMMB nesting
Resolution	**0.7x0.5 deg**	0.1x0.1 deg 0.03x0.03 deg	0.1x0.1 / 0.04x0.04 / 0.01 x0.01
levels	**48**	40 60-70	30 60-70
DA	LETKF	LETKF	NA LETKF
Assimilated Obs	MODIS DT+DB (DU) MODIS DT+DB (ALL)	MODIS DT+DB (DU)	NA MODIS DT+DB (ALL)
Aerosol Species	***DU, SS, BC, POA, SOA bio,*** SOA anthro, SOA fires, ***SU,*** NI	DU	CMAQ (AERO5) MONARCH aerosols
Gas phase chemistry	CBM-IV CB05 ONLINE and ***CLIMATOLOGY***		CB05 CB05
Emissions	***HERMESv3 (HTAP v2)*** ***MEGAN ONLINE***		EMEP, MEGAN / HERMES, MEGAN/ HERMES MEGAN
Bio. Burn. Emissions	***GFAS NRT***		NA GFAS NRT

Developments

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Extending the flexibility of chemistry solvers in MONARCH: Chemi More (Matt Dawson)

- Change the chemical mechanism ***without recompiling***
  - Vary mechanism complexity based on conditions/location
  - Compare mechanisms in real time
- Use ***same mechanisms*** across models (MONARCH, PartMC, etc.) changing only Aerosol Representation JSON



ACRONNiM

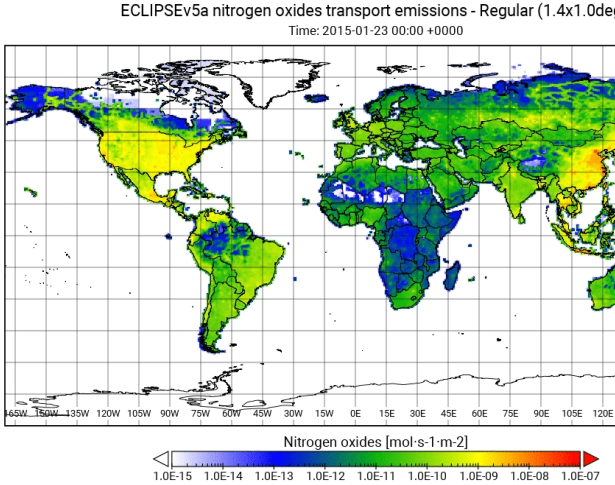
BROWNING

The PartMC library is available at: `https://github.com/compdyn/partmc`

HERMESv3: The High-Elective Resolution Modelling Emissions System

A **python-based, parallel, open source and multiscale** emission modelling framework that **processes and estimates gas and aerosol emissions** for use in atmospheric chemistry models.

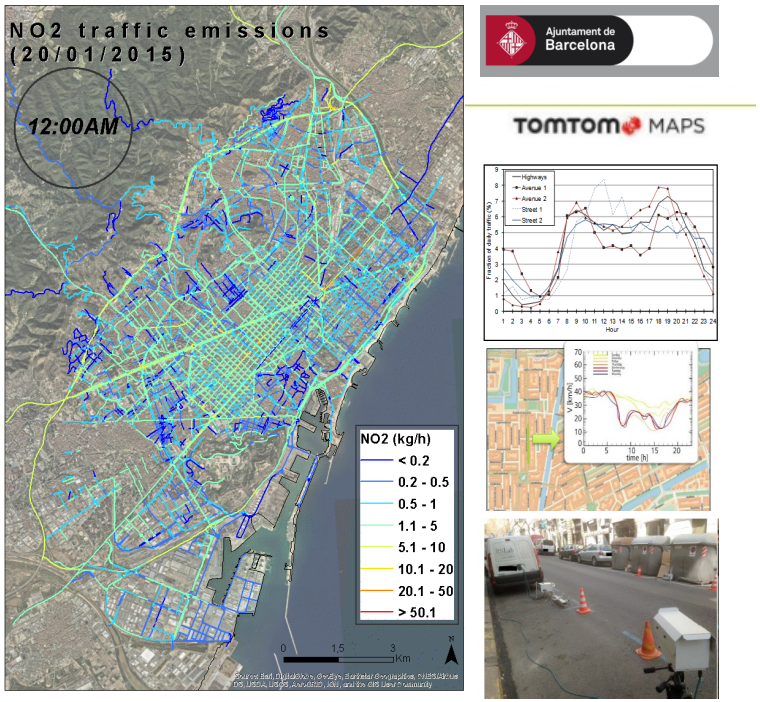
global-regional module (HERMESv3_GR)



https://earth.bsc.es/gitlab/es/hermesv3_gr

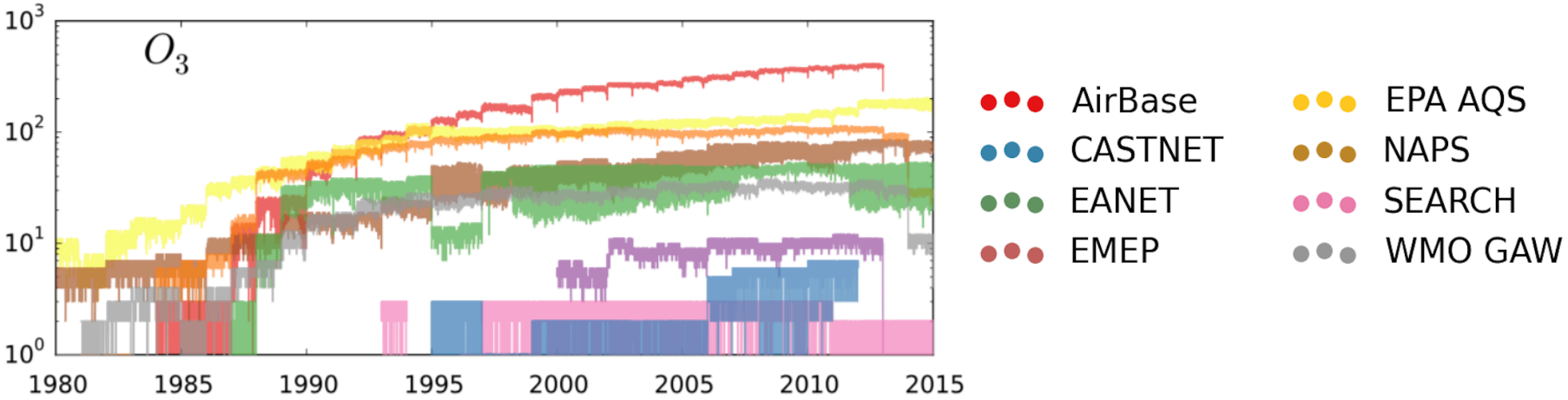
Guevara et al. (2019, GMD)

bottom-up module (HERMESv3_BU)



GHOST: Globally Harmonised Observational Surface Treatment

- With time, more and more observations from different reporting networks are becoming available to the atmospheric chemistry community.



- GHOST provides a framework for the harmonisation of an exhaustive number of data/metadata fields that may provide some use to scientists when using the observations in analyses.

Projects

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

BSC contribution to CAMS

Copernicus Atmosphere Monitoring Service (CAMS) is one of six services that form Copernicus, the European Union's Earth observation programme.

CAMS is implemented by ECMWF on behalf of the European Commission.

- CAMS_84 Phase I and II: Validation – Dust in the Mediterranean
- CAMS_81: Global and Regional emissions – Service evolution on temporal profiles
- CAMS_50 Phase II: Regional production – MONARCH Candidate model
- CAMS_43 Phase II: Global aerosol development - Shortwave radiance assimilation
- CAMS_95: Aircraft Support and Maintenance Service – Dust forecasts

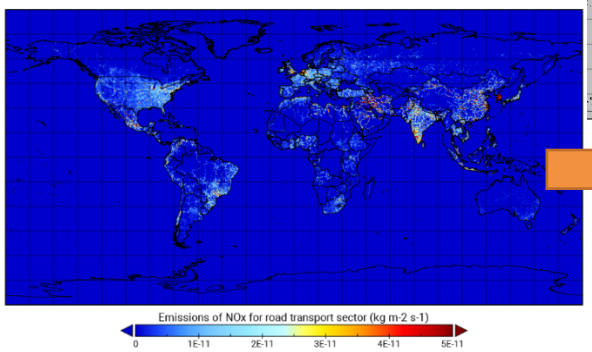
CAMS-81: new temporal profiles

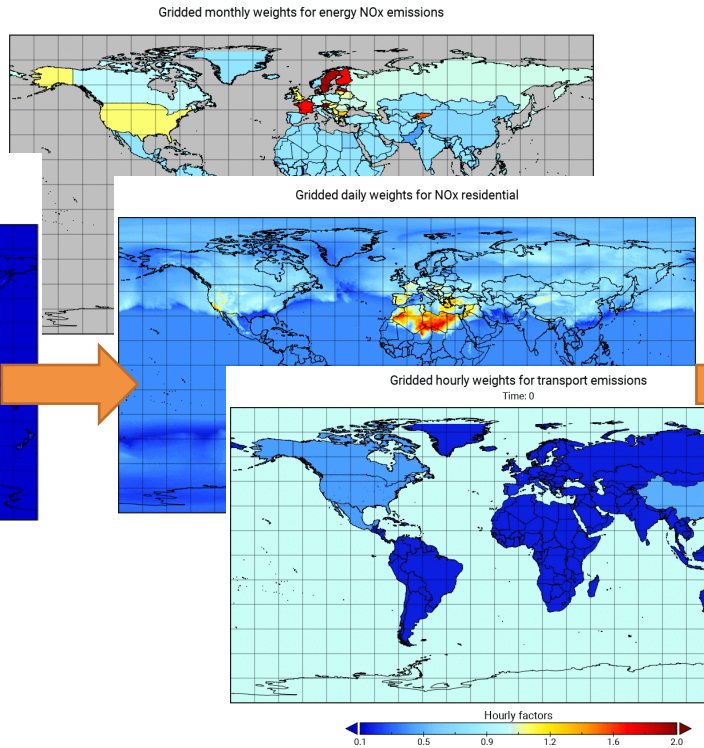
Development of gridded temporal profiles that take into account differences across:

- Sources (energy and manufacturing industry, residential combustion, traffic and agriculture)
- Countries and regions (climatological and sociodemographic aspects)
- Pollutants (NO_x, CO, NMVOC, NH_3, SO_x, PM_{10}, $PM_{2.5}$, CO_2 and CH_4)

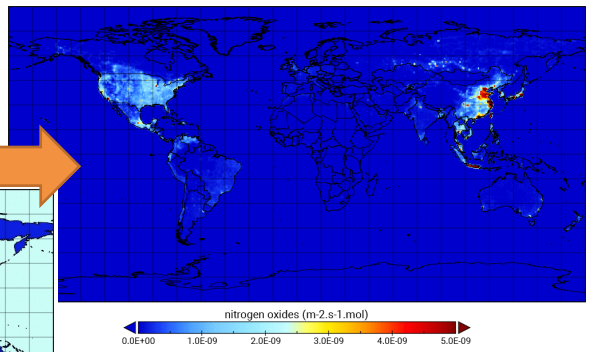
Monthly, daily, weekly and hourly profiles

Annual emissions





Hourly emissions



Soon publicly available through the ECCAD system (https://eccad.aeris-data.fr/)

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Copernicus Europe's eyes on Earth

Atmosphere Monitoring Service

CAMS-43: WP3 on SW radiance data assimilation

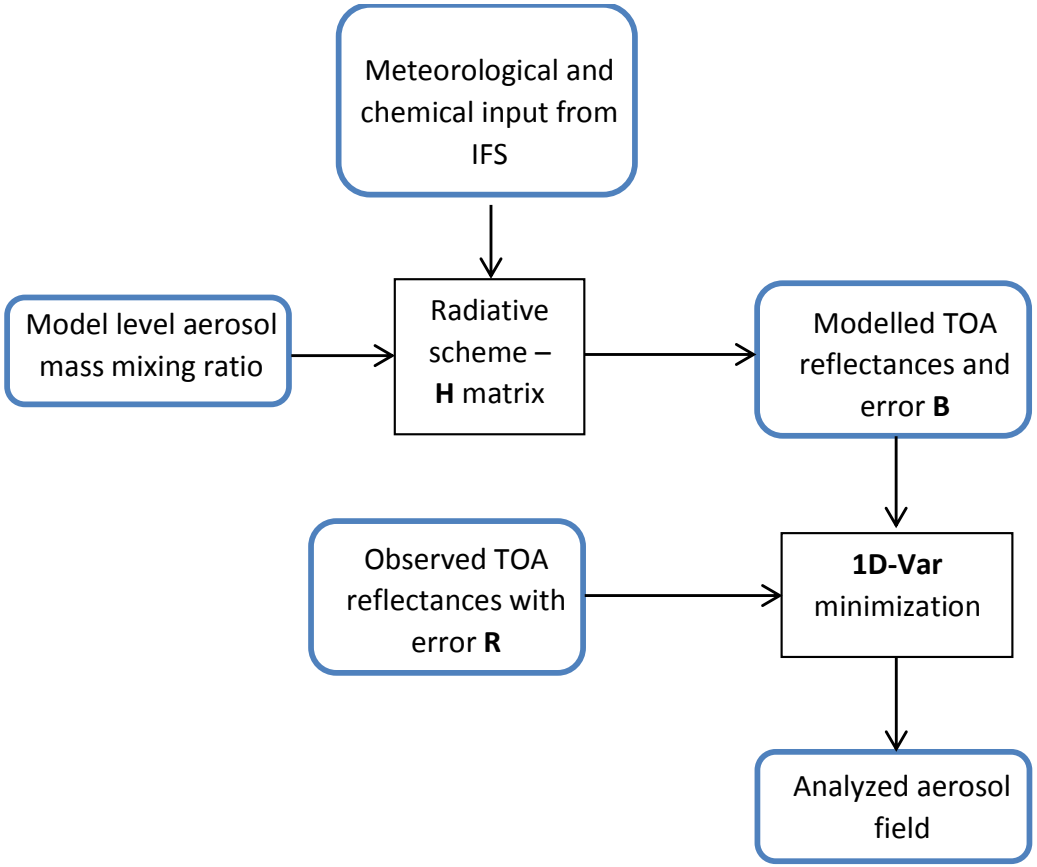
Simple 1D-Var code

Shortwave radiative transfer models:
- CDISORT, DISORT, FLOTSAM (implementation in the 1DVar in development)

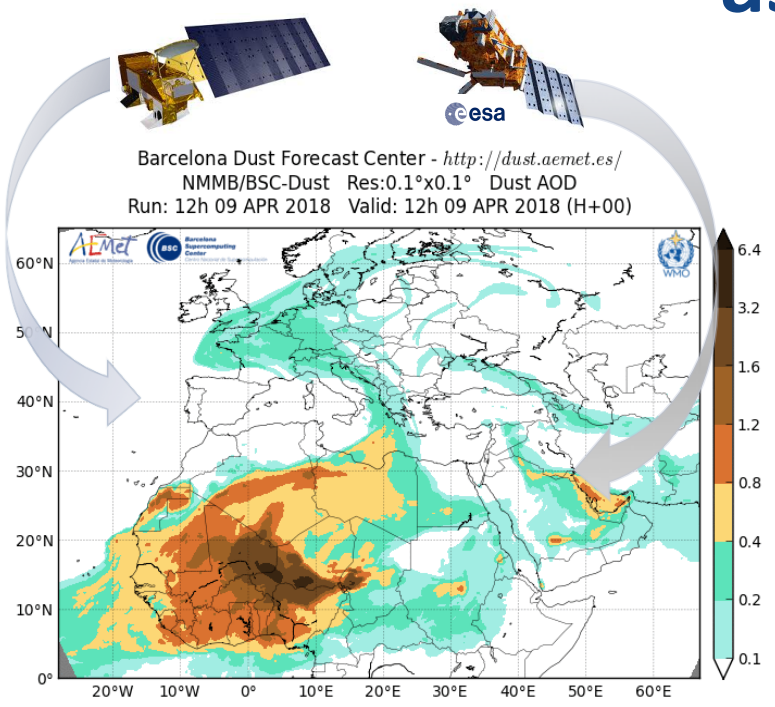
Which variables to control?
- AOD per aerosol type
- AOD vertical profiles
- Aerosol size distributions
- Surface reflectance

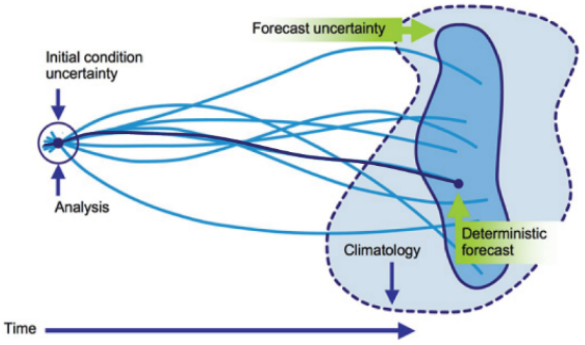
Observations:
- How many viewing geometries and wavelengths are needed?
- Limits on the observational errors?

Testing:
- Test with synthetic radiance observations
- Test with real radiance observations

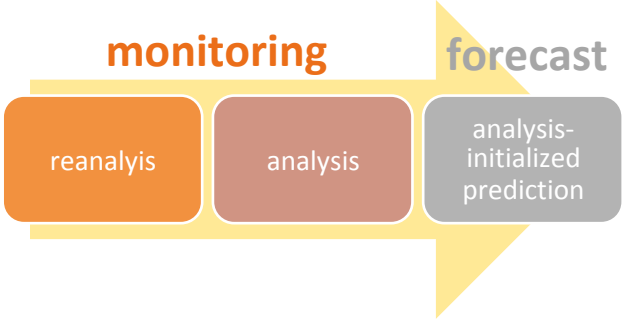


MONARCH ensemble forecast for dust data assimilation

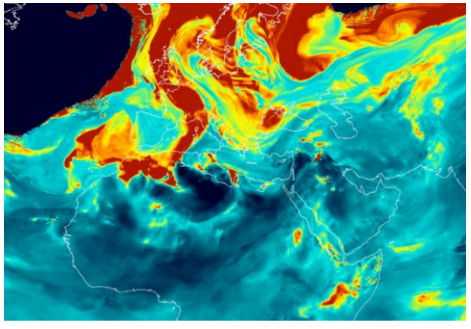




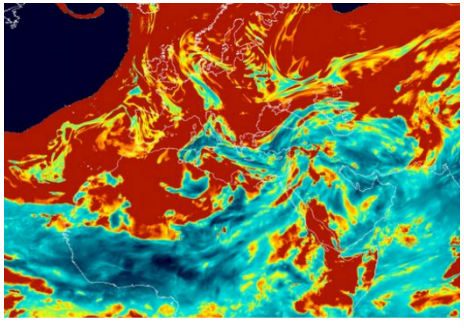
Role of the ensemble:
- spatial spreading of information from observations
- statistically consistent increments between neighbouring grid points
- multivariate analysis



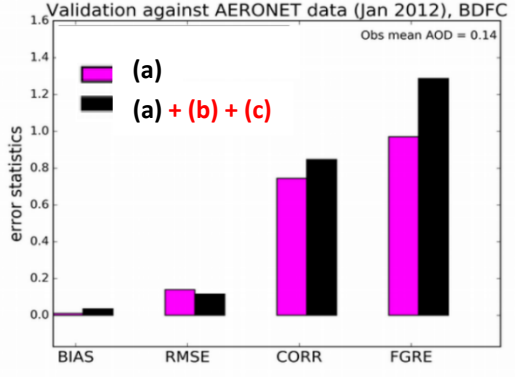
Normalized standard deviation



(a)



(a) + (b) + (c)



(a) multi-parameter source perturbations
(b) multi-physics source perturbations
(c) multi-meteorological initial and boundary conditions

DustClim Project (2017-2020)

DustClim

ERA4CS European Research Area for Climate Services

Produce a **high resolution dust reanalysis** for Northern Africa, Middle East and Europe covering the satellite era of quantitative aerosol information, and develop **dust-related services** tailored to specific socio-economic sectors (**transport, energy, health**)

BSC AEMet Agencia Estatal de Meteorología cnrs

Challenges for CES&AC

high resolution

feasibility

code parallelization & efficiency

multi-year simulations

store & *retrieve*

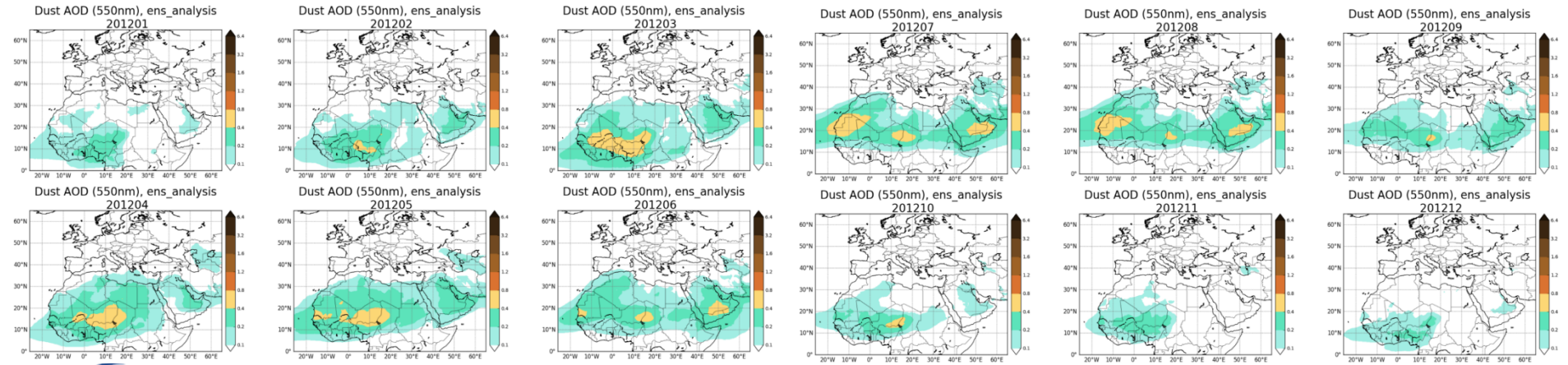
storage conventions & MONARCH_reduce

ensemble simulations

automatisation

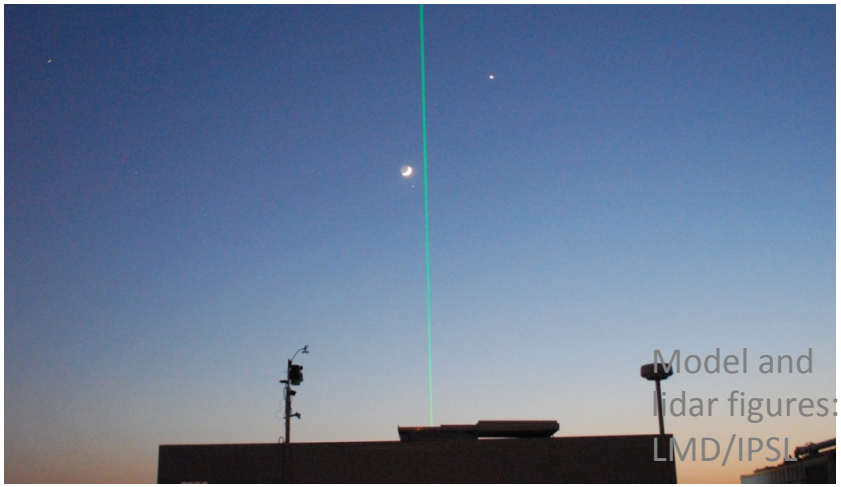
autosubmit & auto-monarch

Monthly dust analyses for 2012

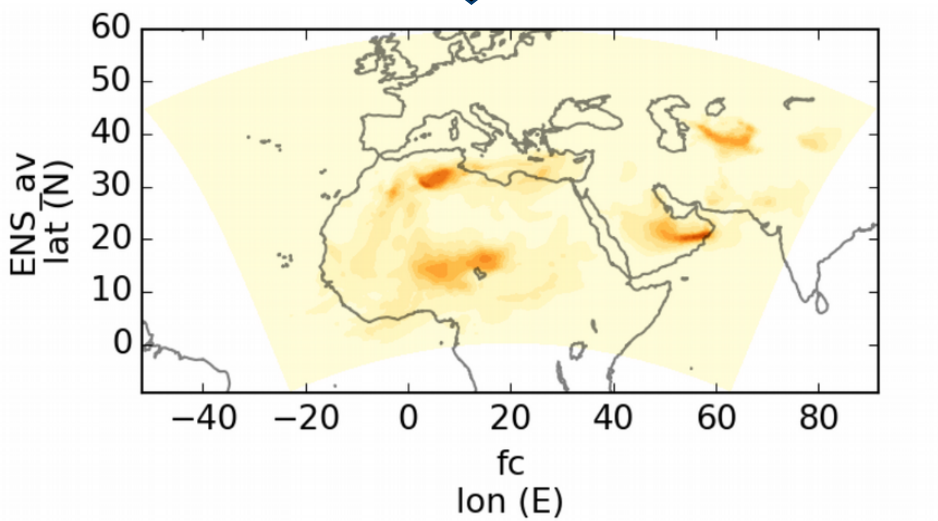


BSC Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Data assimilation of vertical dust profiles (J. Escribano)



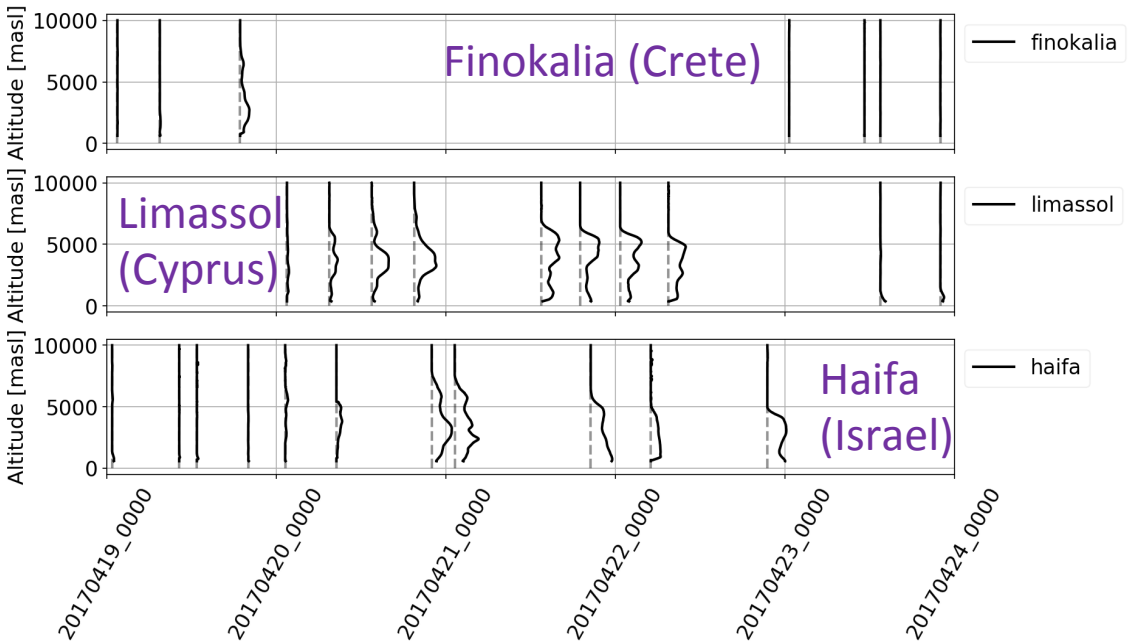
Dust optical depth

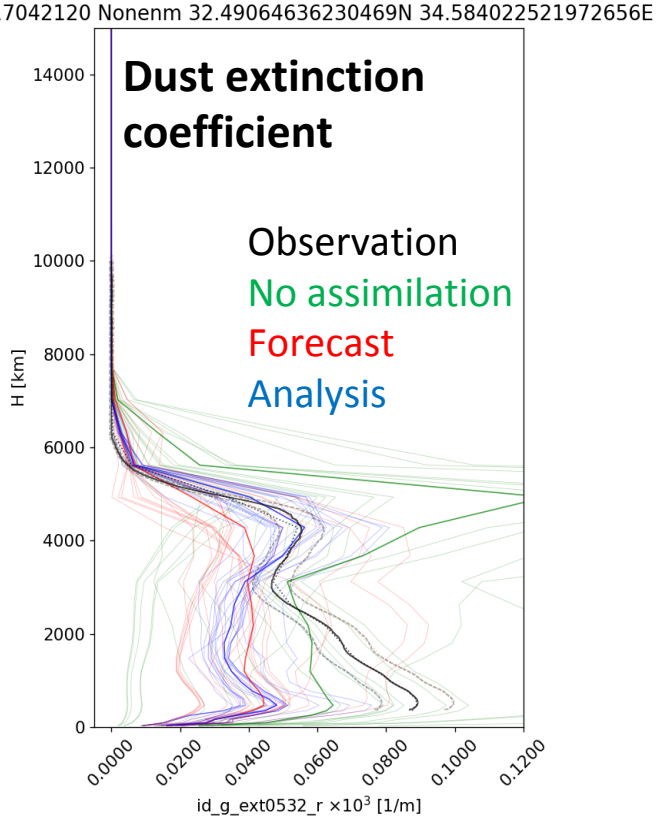


Barcelona Supercomputing Center
Centro Nacional de Supercomputación

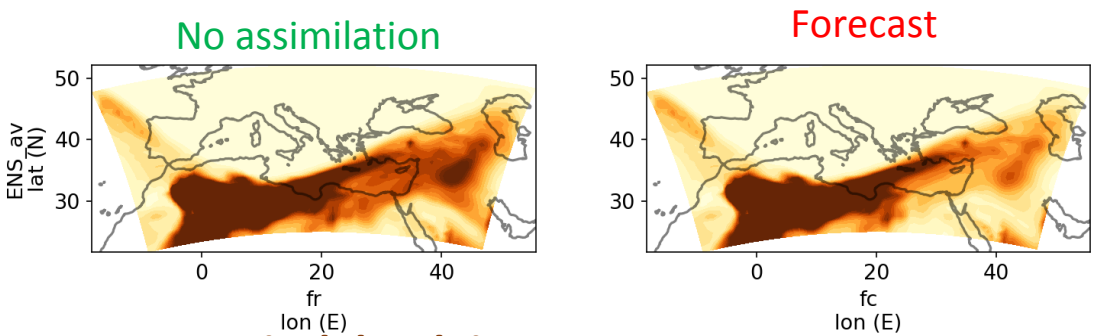
STARS

OBS: Dust extinction coefficient

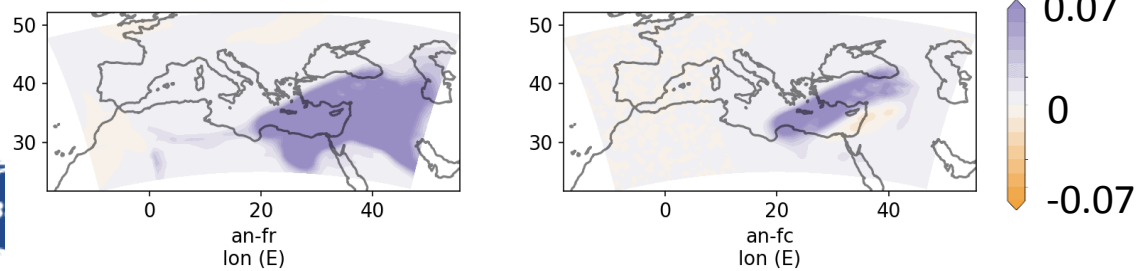




Dust optical depth



Dust optical depth increments

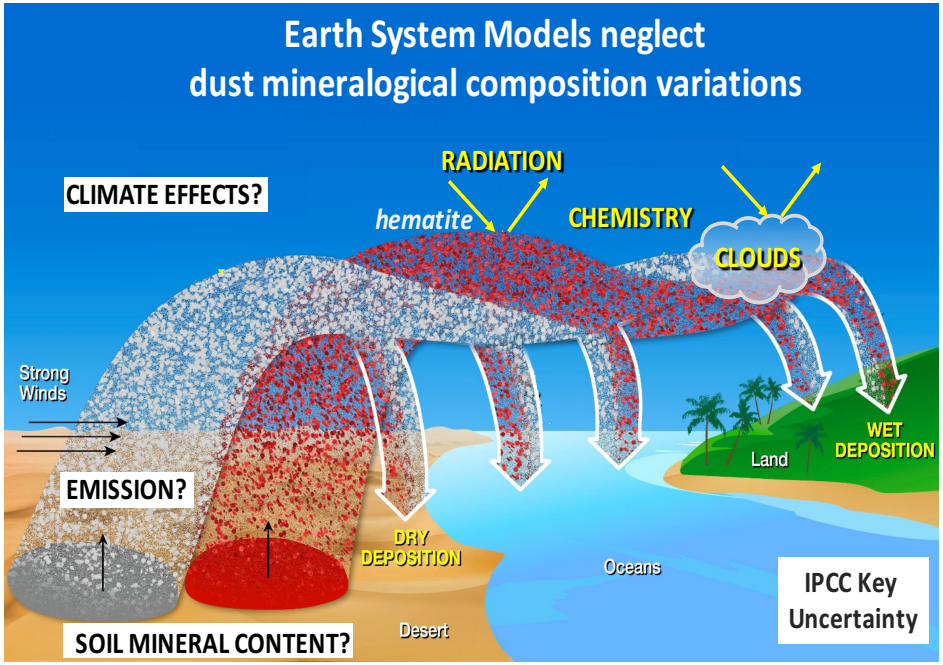


STARS

FRAGMENT: FRontiers in dust minerAloGical coMposition and its Effects upoN climaTe

CONTEXT

- Dust aerosols are a mixture of different minerals, whose relative abundances, particle size distribution (PSD), shape, surface topography and mixing state influence their effect upon climate.
- **Soil mineralogy atlases** for dust modelling are uncertain. They are derived by massively extrapolating an inhomogeneous and limited set of mineralogical analyses of soil samples that are particularly scarce in the arid and semi-arid areas that contain the dust sources
- **Future high quality space borne spectroscopic mapping of soil mineralogy** is a promising path to understand the relative abundance of the key dust source minerals with sufficient detail and coverage, but the use of this resource has been virtually unexplored in the context of dust modelling.
- The complete lack of experimental studies tackling the size-resolved mineralogy of emitted dust due to **fragmentation of soil mineral aggregates** and its relationship with the parent soil hinders our ability to extend and constrain the theories of dust emission used in models.



European Research Council
Established by the European Commission

AXA Research Fund

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

idaea CSIC
Consejo Superior de Investigaciones Científicas

Technische Universität Darmstadt

JPL

NASA
National Aeronautics and Space Administration
Goddard Institute for Space Studies
New York, N.Y.

PSI
Planetary Science Institute

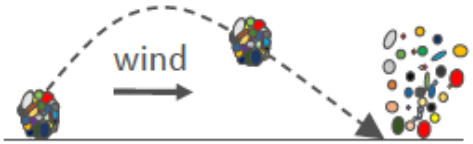
Caltech

Challenges

Methods

Obj1 WP1

Emission of minerals

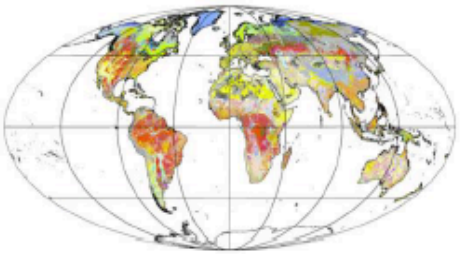


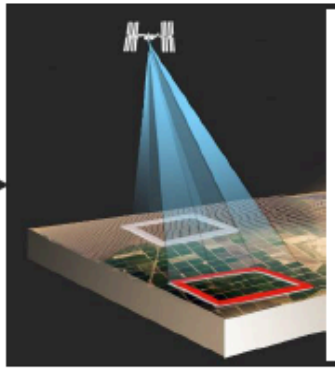
FRAGMENTation of aggregates

Theory
+
field campaigns
+
Laboratory analyses

Obj2 WP2

Global soil mineral content

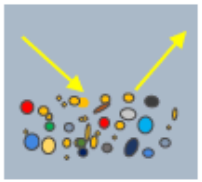


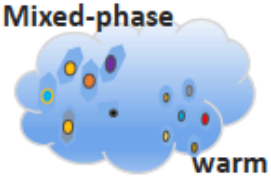


Field and Lab
+
Airborne spectroscopy
+
Space-borne spectroscopy
EMIT

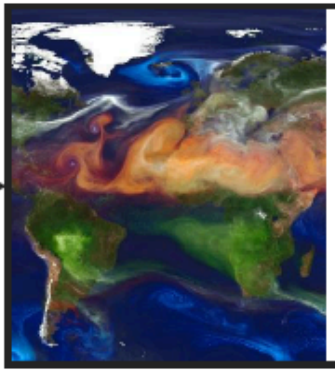
Obj3 WP3

Role of mineralogy





Radiation, Chemistry and Clouds



Modelling
+
State-of-the-art
+
New methodologies
EMIT

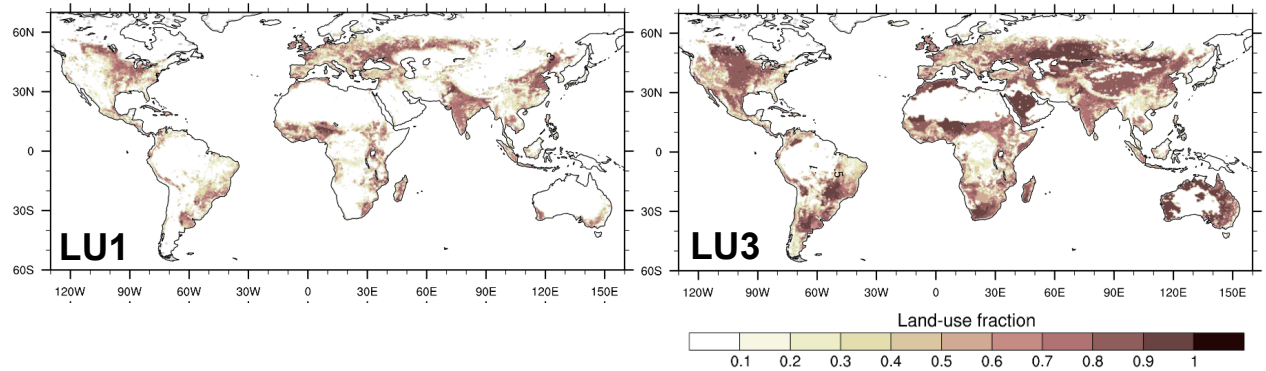
Barcelona Supercomputing Center
Centro Nacional de Supercomputación
European Research Council
Established by the European Commission
AXA Research Fund

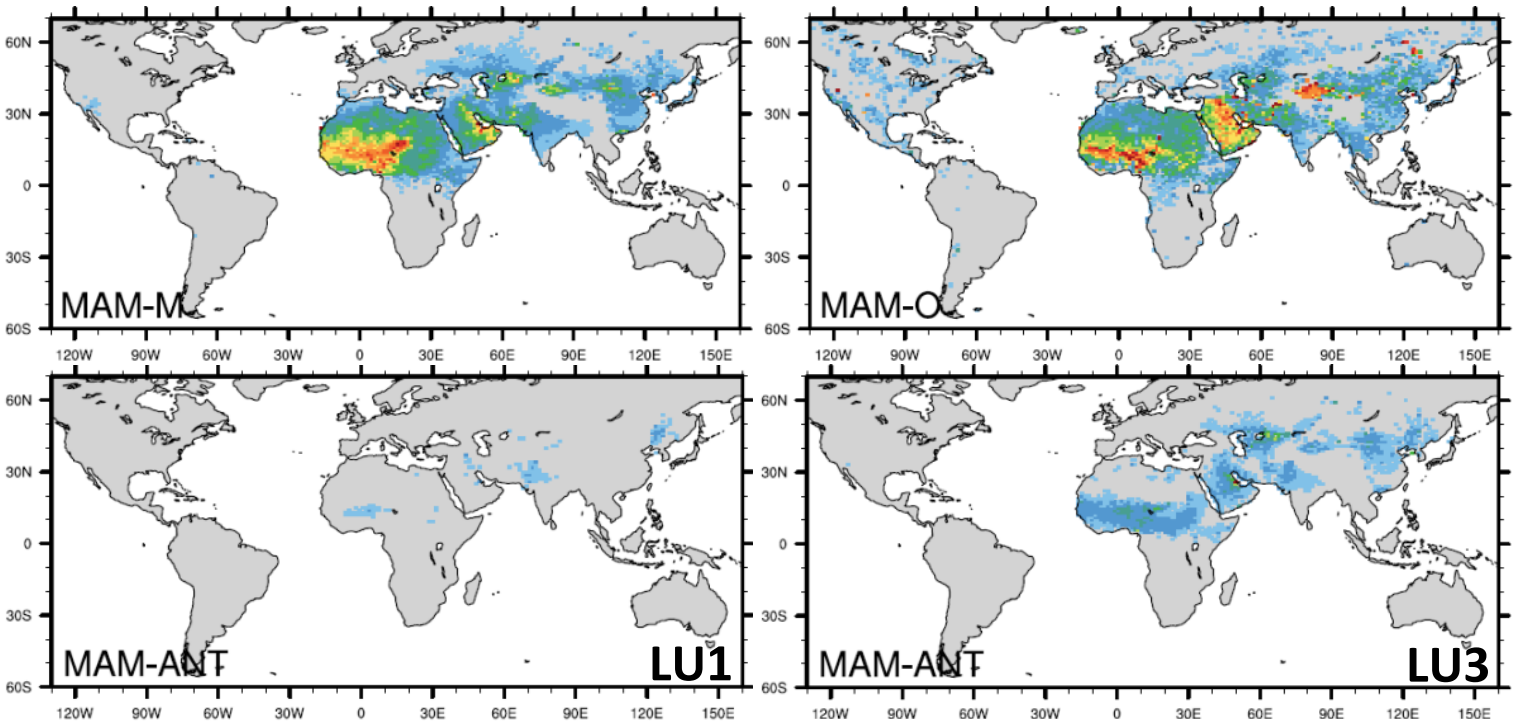
Dust emission from natural and anthropogenic sources (M. Klose)

Land-use scenarios:

(**LU1**) Cropland, pasture

(**LU3**) Cropland, pasture, converted rangeland, rangeland





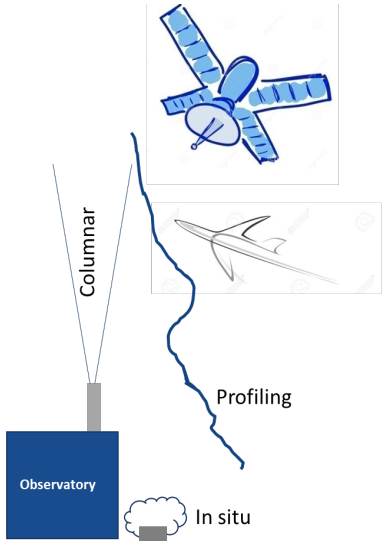
DUST.ES

Klose et al., in prep.

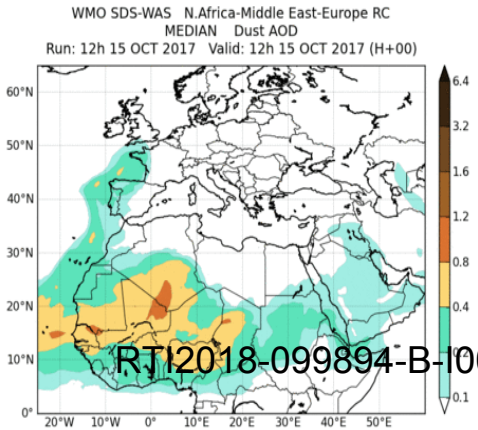
SDS-WAS Regional Center activities

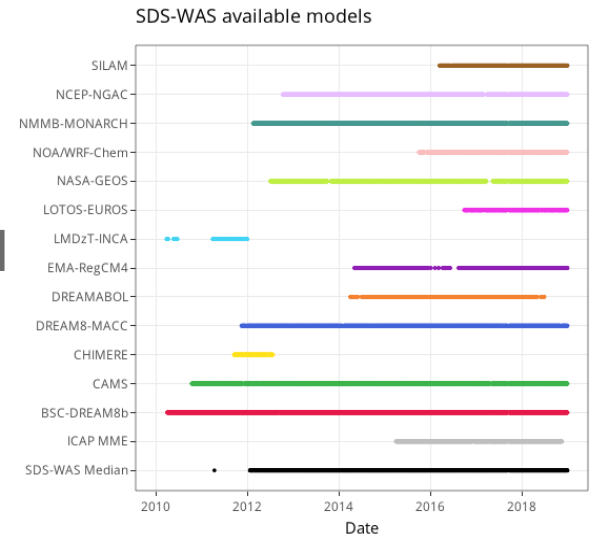
Harmonised storage of observations and forecasts

NRT Observations



Unique dust 72h forecast ensemble based on 12 models

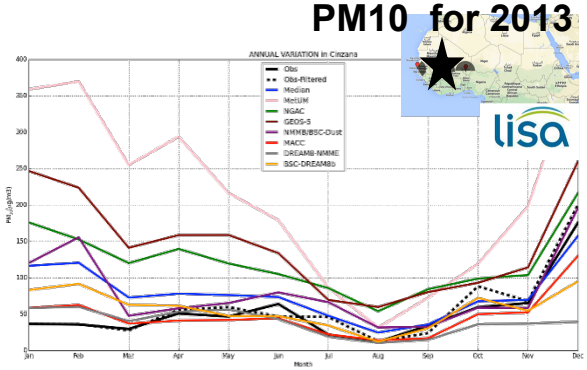




RTI2018-099894-B-I00

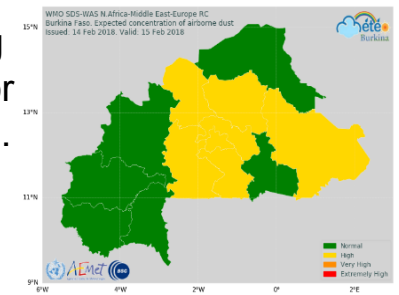
Model evaluation: Dust-filtered observations are used to provide the performance of the models

PM10 for 2013



User-oriented products: Warning Advisory System for Burkina Faso and… in the future for NAMEE

inDust



Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Agencia Estatal de Meteorología

http://sds-was.aemet.es/

18th AeroCom workshop

7th AeroSAT workshop

September 23 – 28, 2019
BSC, Barcelona, Spain

hosts: **Carlos Perez and Alexis Chanthasak**
carlos.perez@bsc.es alexis.chanthasack@bsc.es

co-organizers (AeroCom): Michael Schulz / Stefan Kinne / Mian Chin
co-organizers (AeroSAT): Thomas Popp / Ralph Kahn

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Deadline registration **1st August**

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

EXCELENCIA SEVERO OCHOA

Thank you!

Acknowledgments

- European Research Council Grant FRAGMENT
- Ministerio de Economía y Competitividad (MINECO) as part of the BROWNING project RTI2018-099894-B-I00
- European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 747048, 789630 and COFUND-2016-754433
- Copernicus Atmosphere Monitoring Service (CAMS)
- ERA4CS

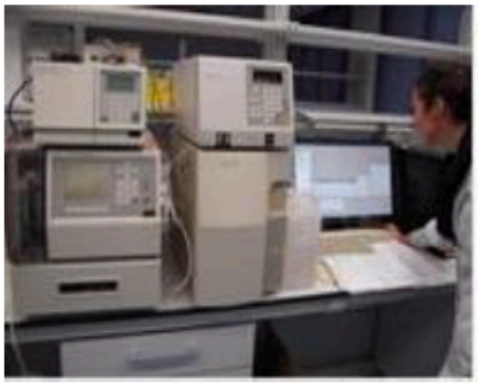
11th ICAP WG meeting - Tsukuba (Japan)

22/07/2019

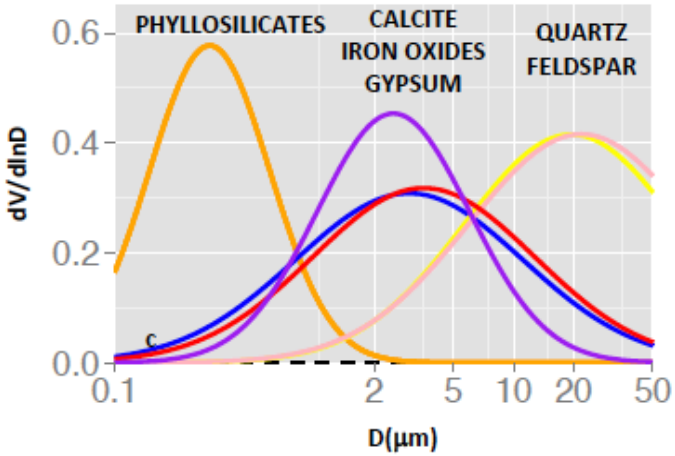
FRAGMENTation of aggregates

Understand emitted PSD of minerals and relationship with parent soil
Extend theoretical framework(s) and produce global model scheme

Field campaigns



Laboratory



Theory
Hypotheses testing

- Spain, Morocco, US and *Iceland*
- Atmospheric Forcing
- Size-segregated and composition resolved dust fluxes
- Size-segregated and composition resolved dry and wet soil

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

European Research Council
Established by the European Commission

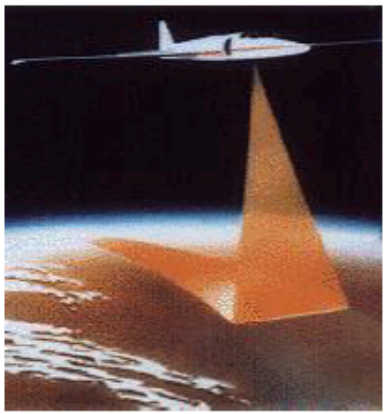
AXA Research Fund

Global soil-surface mineralogy

Constrain global soil-surface mineralogy
Link spectroscopy of soil to dust emission

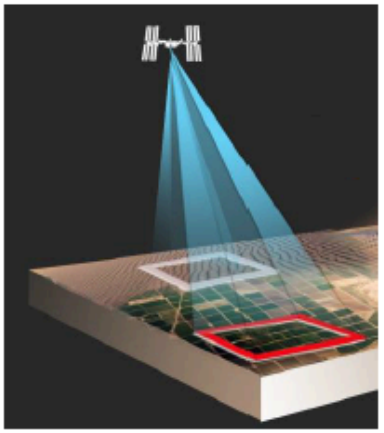
Field and lab spectroscopy

AVIRIS (US)



Airborne Spectroscopy

HYPERION/EMIT (2021)



Space-borne Spectroscopy

- Spain, Morocco, US….
- Point and field spectrometers
- Spectroscopy of soil and Aeolian samples
- Tetracorder Spectral Identification and Mapping
- Linking to size and composition resolved measurements relevant to theories of dust PSD

SUPPORT and TIMELY IMPACT EMIT

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

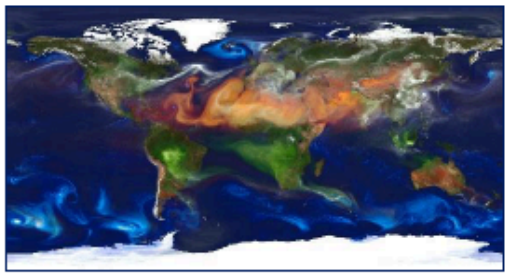
European Research Council
Established by the European Commission

AXA Research Fund

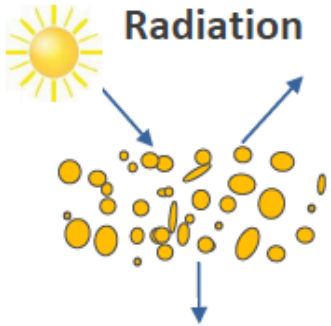
Modeling and effects

Quantify the present-day dust direct and indirect radiative forcing
Minimal representation of mineralogy in Earth System models

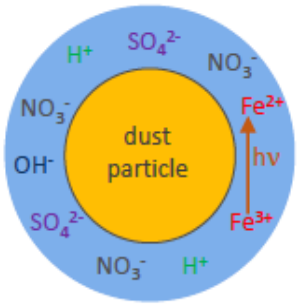
Modeling



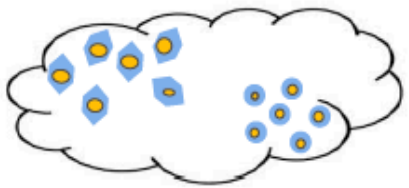
EMIT models
AEROCOM-like experiments



Heterogeneous Chemistry



Clouds



- BSC MONARCH Model
- Co-development with GISS ModelE
- Model constrained by new PSD's and mineral maps
- Data assimilation and thorough model evaluation
- Modeling optical properties (shape and mineralogy)
- Further constraints with radiance measurements
- Using state-of-the-art schemes for chemistry and clouds

Barcelona Supercomputing Center
Centro Nacional de Supercomputación
European Research Council
Established by the European Commission
AXA Research Fund